checkCIF/PLATON report

Structure factors have been supplied for datablock(s) er078_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: er078_sq

Bond precision: C-C = 0.0062 A Wavelength=0.71073

Cell: a=13.4894(6) b=14.8036(6) c=17.0021(6)
alpha=64.769(4) beta=73.282(4) gamma=86.538(4)
Temperature: 150 K

	Calculated	Reported
Volume	2933.9(2)	2933.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C73 H63 Li4 N13 O41 Zn4 [+ solvent]	?
Sum formula	C73 H63 Li4 N13 O41 Zn4 [+ solvent]	C88 H98 Li4 N18 O46 Zn4
Mr	2067.69	2433.08
Dx,g cm-3	1.170	1.377
Z	1	1
Mu (mm-1)	0.883	0.899
F000	1052.0	1252.0
F000’	1053.69	
h,k,lmax	18,20,23	18,18,22
Nref	15601	12851
Tmin,Tmax	0.744,0.956	0.747,1.000
Tmin’	0.729	

Correction method= # Reported T Limits: Tmin=0.747 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.824 Theta(max)= 28.999

R(reflections)= 0.0633(9028) wR2(reflections)= 0.2064(12851)

S = 1.067 Npar= 697

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  N   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.9 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Zn1 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00625 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.721 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        15 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C88 H98 Li4 N18 O46 Zn4
           Atom count from the _atom_site data:  C73 H63 Li4 N13 O41 Zn4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    1
          From the CIF: _chemical_formula_sum  C88 H98 Li4 N18 O46 Zn4
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         88.00     73.00   15.00
          H         98.00     63.00   35.00
          Li         4.00      4.00    0.00
          N         18.00     13.00    5.00
          O         46.00     41.00    5.00
          Zn         4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        21 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        34 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ    Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.004 Degree
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records         2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         7 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         5 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1D        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1D        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11D       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12D       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13D       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11D       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12C       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at       0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        17% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C12D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C13D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C22D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C23D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C32D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C33D Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H12B     ..H23A     .       1.73 Ang.
                                                  1+x,y,z  =      1_655 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        309 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       2555 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          7 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.0 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ           2 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  44 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  26 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock er078_sq - ellipsoid plot